

Connecting electronic structure with inter-atomic potentials: Si(111)5x2-Au

Jessica McChesney
University of Wisconsin

One-dimensional systems are predicted to exhibit a variety of exotic phenomena as a result of the fundamental electronic and structural differences with higher-dimensional systems. Specifically, low-dimensional systems are susceptible to a variety of instabilities. Connections between electronic and structural instabilities were explored by investigating of the Si(111)5x2-Au surface reconstruction. The 5x2 surface is comprised of an underlying 5x2 chain and a 5x4 dopant superlattice. Recent first-principles total energy calculations determined that the optimal doping corresponds to one adatom per 5x8 unit cell; however, instead of an ordered 5x8 lattice a disordered, half-filled 5x4 lattice is observed experimentally. The deviation from the expected 5x8 superlattice to a phase-separated structure is the result of instabilities at the Fermi surface (nesting of the Fermi lines that sit at the zone boundary of a 5x4 unit cell). Mapping of the band structure via angle-resolved photoemission reveals three distinct bands. The first is completely below the Fermi level and, therefore, does not contribute significantly to the formation of instabilities. The other two bands lie near E_F and are prime candidates for triggering the 5x4 superlattice formation since both approach E_F at the zone boundaries of a 5x4 unit cell. One band is observed to be metallic, and the other band is semiconducting. It is the competition between the 5x4 potential that is favored by the electronic structure and the doping by the Si adatoms which leads to this phase separation.